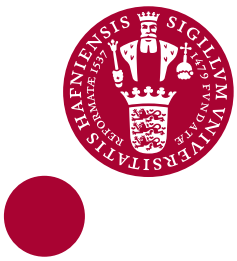

RPA(D) and HRPA(D): 13C-13C Spin-Spin Coupling Constants for Saturated Cycloalkanes

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RPA(D) and HRPA(D): ^{13}C-^{13}C Spin-Spin Coupling Constants for Saturated Cycloalkanes

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Abstract

This study investigates the performance of the SOPPA-based, doubles-corrected methods RPA(D) and HRPA(D) in calculating carbon-carbon spin-spin coupling constants in 39 saturated carbocycles, totaling 188 unique coupling constants. RPA(D) scales an order below SOPPA in computational complexity while HRPA(D) differs from SOPPA in the leading coefficient. These methods may therefore prove beneficial in predictions of coupling constants of large molecules. It was found that HRPA(D) significantly improves on RPA(D) for all coupling constants as well as performing similarly to SOPPA in terms of accuracy. With a roughly 50% reduction in computation time from SOPPA to HRPA(D), the latter shows great promise for the calculation of nuclear indirect carbon-carbon spin-spin coupling constants in saturated carbocycles.